INSTITUTIONAL COMPUTING AT LOS ALAMOS

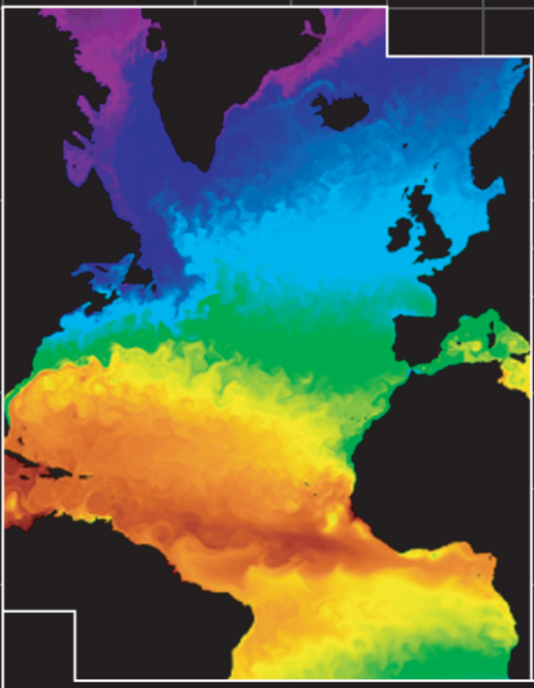
PROVIDING TOOLS FOR BETTER DECISIONS

Computing has been an exciting part of Los Alamos since the days of the Manhattan Project. Bolstered by a rich legacy of resources—from the MANIAC, the Cray-1, and Thinking Machines' CM-5 to the Blue Mountain and Q machines—Los Alamos is working to achieve its goal of science-based prediction.

Computational science at Los Alamos, therefore, combines observations and data with models and theory to simulate the future, the past, and the workings of both the cosmically large and the infinitesimally small. Using the same technology, we can predict what will happen in climate, wildlife, and water resources; watch the meteor impact that killed the dinosaurs during the late Cretaceous Period; and examine both the structure of the Universe and the machinery within our own cells.

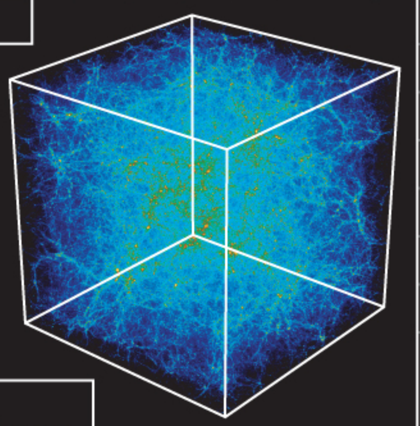
Predicting the future is about making better decisions and providing everyone with a better understanding of how the choices we make affect the future. For example, knowledge about changes in rainfall patterns and forecasts of water resources can be used to encourage conservation during long-term scarcity and to reduce flood damage during short-term abundance. Understanding the effects of fossil fuels and the risks of nuclear power can lead to a greater appreciation of available alternatives.

Thus, Los Alamos is taking on a new challenge, building computational tools to examine situations that extend far beyond the classic scientific method. Perhaps most important, we must provide the tools for managing, analyzing, and verifying the predictive tools themselves.



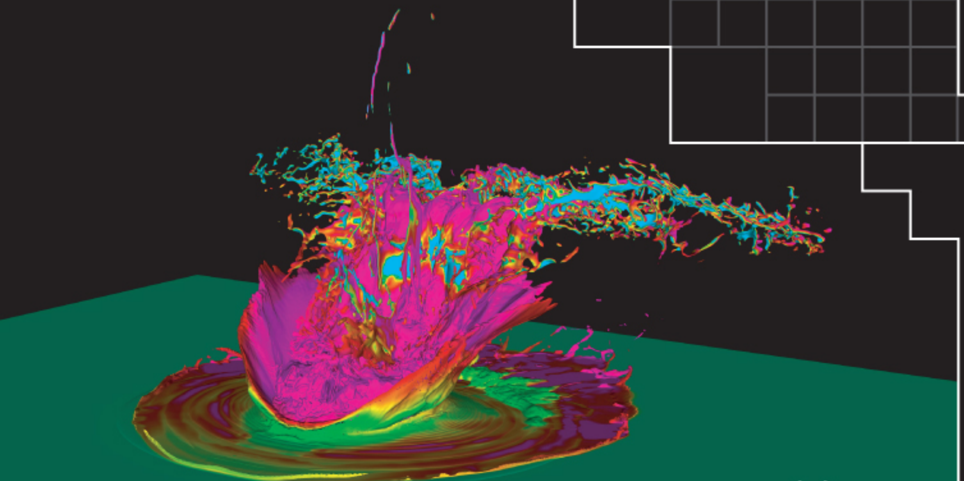
sea-surface temperature

This snapshot of sea-surface temperature is from a simulation of the North Atlantic Ocean by the Los Alamos Parallel Ocean Program. The computational-grid resolution is 0.1° (10 kilometers at the Equator) in latitude and longitude, with 40 depth levels. Red indicates the warmest water. The Gulf Stream moves polarward along the east coast of North America. This simulation shows our ability to reproduce the present state of the ocean and is also one component of a complete climate model, which can be used for climate predictions.



cosmologic structure

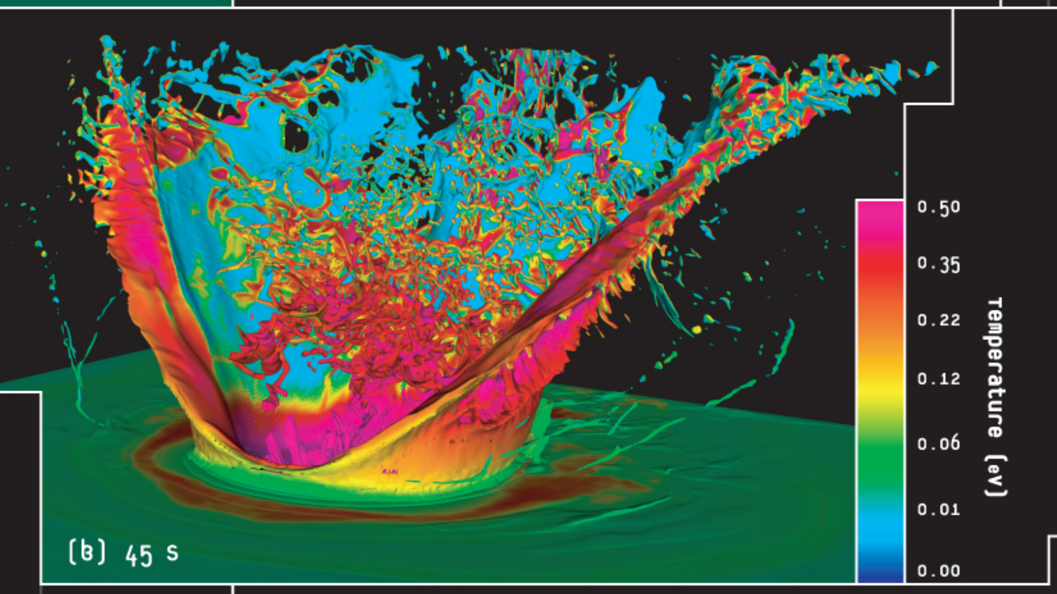
This image represents a portion of the Universe about one billion light-years across. Scientists can probe the origin of the large-scale structure and the evolution of the Universe by picking a set of cosmologic parameters, modeling the growth of structure, and then comparing the model with the observations.



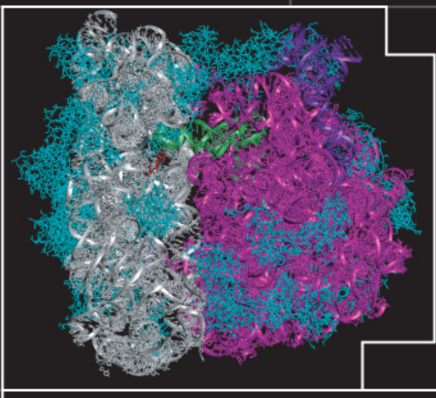
(a) 11 s

simulations of a meteor impact

These simulations show a 10-kilometer-diameter asteroid striking Earth 65 million years ago during the late Cretaceous Period. **(a)** A few seconds after impact, billions of tons of hot material are lofted into the atmosphere. **(b)** Less than a minute after impact, dissipating energy produces an explosion that melts, vaporizes, and ejects large amounts of calcite, granite, and water from the site. **(c)** Two minutes after impact, the debris curtain has separated from the rim of the still-forming crater as material in the curtain falls to Earth in a blanket of ejecta that is asymmetric around the crater.

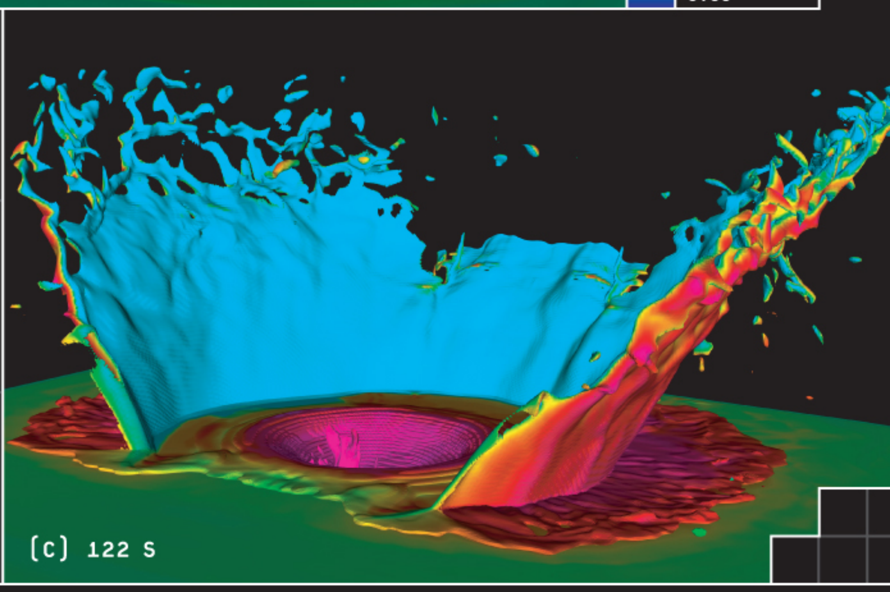


(b) 45 s



The Ribosome in Motion: Simulating the CPU of the Cell

Large-scale simulations of the 70S ribosome have set a new state of the art in biomolecular simulation. The ribosome is an ancient molecular "machine" responsible for translating the genetic code in all living things. The initial structure of the simulation was developed by an advanced RNA motif homology effort, led by Chang-Shung Tung.



(c) 122 s

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